Energy Dissipation to Defect Evolution (EDDE)
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Lead Institution: Oak Ridge National Laboratory
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Mission Statement*: To develop a fundamental understanding of energy dissipation mechanisms in tunable concentrated solid-solution alloys, and ultimately control defect evolution at the early stage in a radiation environment; and to yield new design principles and accelerate science-based material discovery of radiation–tolerant structural alloys for energy applications.*

Approaches for improving the performance of structural materials have been intensively investigated for many decades due to their importance in many applications. Solid solution strengthening, traditionally by alloying minor elements into pure metals, is one of the most widely used methods to achieve specific desirable properties, including radiation tolerance. While it has long been recognized that specific compositions in binary and some ternary alloys have enhanced radiation resistance, it remains unclear how the atomic structure and chemistry affect defect formation and damage evolution. This project directly addresses this knowledge gap in order to enable future-generation energy technologies.

The evolution of radiation–induced defect concentration in alloys can be described by three simplified competing processes (Fig. 1): defect production from collision cascades (1st term), vacancy–interstitial recombination within the diffusion volume during the cascade events (2nd term), and extended defect cluster formation from the accumulation of the cascade damage and absorption of point defects by nano-scale features (sinks) such as additional phases, interfaces, grain boundaries, and precipitates (3rd term). The first two terms are short-time processes up to a few picoseconds, while the 3rd term includes the processes over a much longer time scale. Localized atomic displacements from direct knock-on processes have long been considered to dominate the formation of defects. The work here examines the hypothesis that electronic excitations, heat flow, and the interaction between these may be critical, and that a fundamental understanding of roles of electrons, phonons, and magnons in energy dissipation is necessary for the developing new materials.

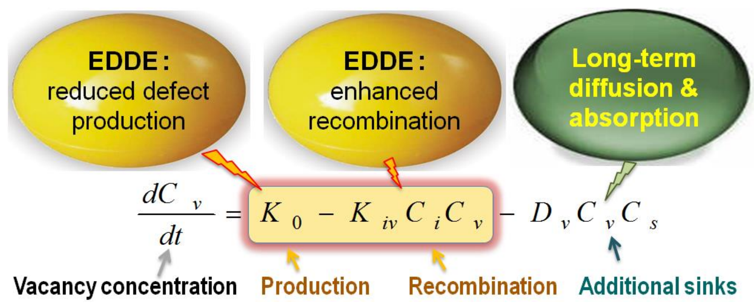

Fig. 1 Simplified terms showing competing processes controlling radiation–induced vacancy concentration. K_0 is the defect production rate; K_{iv} the recombination rate coefficient; and C_i, C_v, D_v and C_s the interstitial and vacancy concentration, the vacancy–sink coefficient, and the sink density; respectively. Similar equations hold for interstitials and other defects.

A new class of materials shows great promise, and may be synthesized with atomic-level control: Single–Phase Concentrated Solid Solution Alloys (SP–CSAs) containing two to five or more multiple principal elements. Two distinctive intrinsic properties are expected: (1) disordered local chemical environments that significantly enhance electron scattering that affects energy dissipation processes, and (2) unique site-to-site lattice distortions that lead to atomic level compressive or tensile stress and complex energy landscapes, which affect defect migration and impart exceptional mechanical properties. To realize the potential of these transformative alloys, we must understand the roles of all constituents in their structural stability and their effects on energy dissipation mechanisms at the level of electrons and atoms. While most current research efforts seek to increase sink density (i.e., 3rd term), we focus on the reduction of damage accumulation by acting on the early stages of radiation effects (i.e., 1st and 2nd terms). In the EDDE Center, we progressively advance alloy complexity from elemental Ni to quinternary SP–CSAs (Fig. 2). The ***overarching goal*** of the EDDE EFRC is to develop a fundamental understanding of how the energy of radiation is dissipated, and ultimately to control defect dynamics and microstructural evolution in structural alloys. Specifically, we seek to understand and quantify the mechanisms of energy dissipation through electronic, vibrational, and magnetic excitation, and how these mechanisms are influenced by alloy complexity.

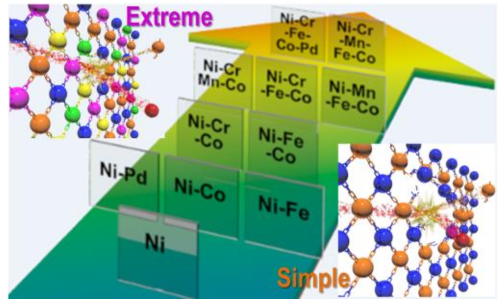

Fig. 2 Increasing complexity in *fcc* single–phase concentrated solid solution alloys.

Two thrusts are designed to test our ***hypothesis*** that modifying alloy complexity will enable us to control defect dynamics at the early stage of radiation damage, which will ultimately allow enhanced radiation tolerance at the later stage under extreme radiation conditions. In Thrust 1, *Energy Dissipation,* we will determine how input energy is partitioned and ultimately dissipated among the electrons and atoms and how these processes are modified by the compositional disorder. In Thrust 2, *Defect Evolution,* we will determine how energy partitioning and energy exchange between the atomic and electronic systems influence the formation, nature and time evolution of defects in irradiated materials, and how compositional complexity alters defect processes. We will also take advantage of recent theoretical and computational developments, many of which were made by members of our Center, to explore for the first time a comprehensive electronic and atomic description of an irradiated material very far from equilibrium. The combination of state-of-the-art experiments and multi-scale computational approaches will offer the possibility to develop critical knowledge needed for controlling and engineering the properties and performance of a material at the ultimate scale – that of atoms and electrons.

The EDDE Center engages a diverse mix of principal investigators and key personnel with complementary experience and skills. Most participants contribute to both Thrusts, thus maximizing synergies and coordination. Strong university involvement enhances educational outreach. Success of the EDDE Center will yield new design principles for radiation-tolerant structural alloys for applications in nuclear energy, and new defect engineering paradigms for much broader science and technology.

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